Molecularly Engineered Energy Materials (MEEM)
EFRC Director: Vidvuds Ozolins
Lead Institution: University of California, Los Angeles

Mission Statement: Create an interdisciplinary world-leading research center to design and synthesize revolutionary new materials for sustainable energy generation, storage and greenhouse gas capture based on cheap, abundant molecular building blocks; disseminate knowledge and increase societal awareness of sustainable energy issues through an integrated program of research, education, and outreach.

EFRC will focus on materials that are inherently inexpensive (such as polymers, oxides, metal-organic frameworks), can be easily assembled from intelligently designed building blocks (molecules, nanoparticles, polymers), and have the potential to deliver transformative economic benefits in comparison with the current crystalline- and polycrystalline-based energy technologies. We will conduct systematic studies of the fundamental mechanisms of carrier generation, energy conversion, as well as transport and storage of charge and mass in tunable, architectonically complex materials. Fundamental understanding of these processes will enable rational design, efficient synthesis and effective deployment of novel three-dimensional material architectures for energy applications. Three interrelated research directions where these novel architectures hold great promise for high-reward research have been identified: solar energy generation, electrochemical energy storage, and greenhouse gas capture.

Organic solar cells: We will design and synthesize novel molecules and nanoscale architectures (see e.g. Fig. 1) that can achieve or surpass 10% efficiency goal for organic solar cells. We will learn to control the nanometer-scale structure of conjugated polymers and polymer blends through the synthesis of novel materials and the use self-assembly techniques, with the goal of producing optimal nanometer-scale structures for photovoltaic applications. Another major goal is to understand how the nanometer-scale structure of conjugated polymer blends controls charge separation, carrier transport, carrier recombination and carrier extraction at the electrodes in working solar cells from both experimental and theoretical perspectives.

Electrochemical supercapacitors: Fundamentally, we will focus on determining why capacitive storage from metal oxides is much less than theoretical estimates; our working hypothesis is that inefficient charge transport in bulk insulating materials is a crucial bottleneck. We will design hierarchically structured electrode materials that integrate electronic and ionic conduction with

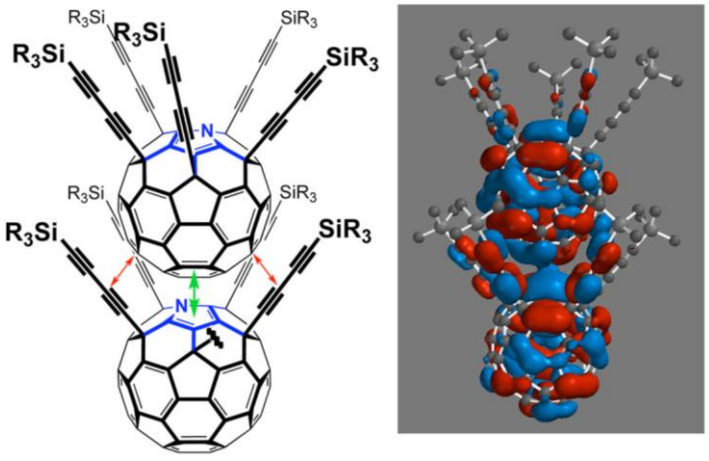

Figure 1. So-called "shuttlecock" molecules based on the heterofullerene $C_{59}N$ with phenyl "feathers" optimized for ideal close contacts within stacks. These molecules are expected to self-assemble into one-dimensional wires, enhancing the efficiency of charge separation and carrier transport in organic solar cells.

pseudocapacitive charge storage. We will also search for new inexpensive materials that combine metallic conductivity with ability for capacitive store charge and explore the efficiency of capacitive charge storage in nanoporous materials using both theoretical and experimental approaches.

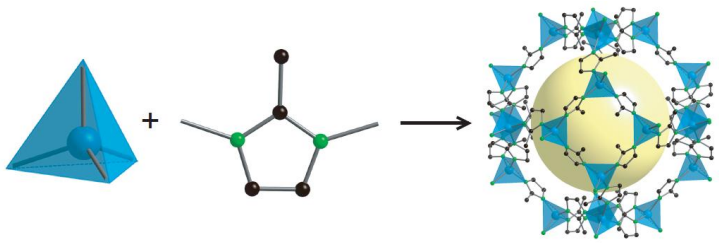

Figure 2: Schematic representation of ZIF formation (ZIF-8, right). ZnN_4 tetrahedra are blue, C, and N atoms are black and green spheres. H atoms are omitted for clarity. The yellow sphere represents the largest sphere that occupies the cavity without contacting the interior van der Waals surface. These materials have been shown to selectively absorb carbon dioxide and other greenhouse gases.

Capturing greenhouse gases: A coordinated effort is proposed for the high-throughput synthesis, characterization and modeling of zeolitic imidazolate frameworks (ZIFs). The structures of ZIFs consist of imidazole groups connected by organic linkers (see Fig. 2) and feature high porosity (2000 m^2/g), high thermal stability (500 °C), and unusually high chemical stability. They have been shown to selectively absorb carbon dioxide and other greenhouse gases. Our research will elucidate the correlation between the structure of a ZIF and its performance, identify the adsorptive sites within the pores of ZIFs, and develop strategies for optimizing the performance of ZIFs to affect highly selective carbon separation.

The three research trusts will be integrated on the basis of common scientific challenges at the fundamental level of electrons, atoms, and molecules: creating innovative nanometer-scale material architectures from custom-designed molecular building blocks to achieve fast, highly efficient charge and mass transfer, and specifically tailored thermodynamics of charge and mass storage.

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University of California, Los Angeles	**V. Ozolins (Director)**, B. N. Dunn (Assistant Director), Y. Lu**,** D. Neuhauser**,** L. Pilon**,** Y. Rubin**,** B. J. Schwartz**,** S. H. Tolbert**,** O. M. Yaghi
University of California at Berkeley	M. D. Asta
University of Kansas	B. Laird
National Renewable Energy Laboratory	N. Kopidakis
Eastern Washington University	Y. Hondonougbo

Contact: Vidvuds Ozolins
Professor of Materials Science & Engineering
Email: vidvuds@ucla.edu
Phone: (310) 267-5538